# On the Evaluation of Accuracy in global tracer transport modeling using the GMI and UCI CTMs

update of Dec 2003 AGU & last GMI talk

Michael Prather & Xin Zhu (UC Irvine) (24 Feb 2004)

- updated Mar 2004 (on GMI / UCI site)
- updated May 2004

Also considerable effort and advice from Jae-Hoon Kim, Dan Bergman (LLNL), Jose Rodriguez (U Miami), & GMI team

### The Transport Part of a CTM:

- a. Tracer transport & mixing
- <u>b. Meteorological Fields</u> ← use the same met fields
- *Transport error* occurs due to numerical approximations in the CTM core (e.g., gridding, flux corrections, advection, boundary layer, convection)
- Take two CTM 'cores' that we expect to have highly accurate tracer transport and hence expect to give similar answers and help us define transport error
- Lin-Rood tpcore: flux-form SLT, stores only tracer mass in each grid cell, calculates high-order polynomial fit for advection (only) and discards after transport, flux corrections to keep positive and eliminate ripples
- Prather SOM: flux-form upstream, stores and uses parabolic fit (second-order moments) to each tracer within each grid cell (9 moments), uses moments for advection, boundary layer, convection, emissions.

### Why fossil-fuel CO<sub>2</sub> as the test case?

Uniform fossil-fuel  $CO_2$  emissions are only one (boring) piece of the atmospheric  $CO_2$  problem and do not begin to address the missing sink, biomass burning signal, ....

#### **BUT**

ff-CO<sub>2</sub> is still the major cause of the North-South gradient in CO<sub>2</sub>. TransCom3 produced similar results for a wide range of CTMs.

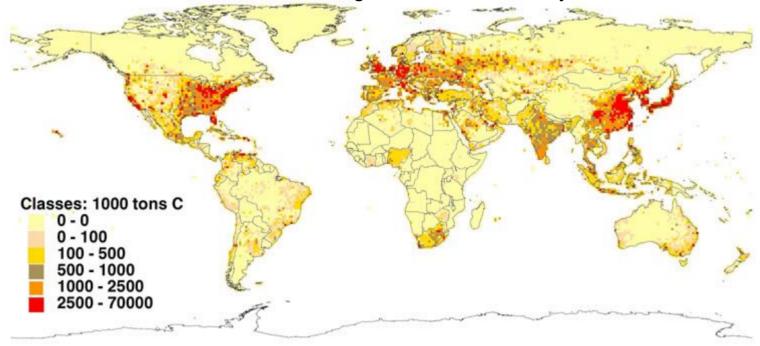
ff-CO<sub>2</sub> is similar to most industrialized emissions (e.g., CFCs in the 1980s, SF<sub>6</sub>) and can be scaled to compare with observed interhemispheric gradients of these species.

A linearly increasing CO<sub>2</sub> abundance (constant 1995 ff-CO<sub>2</sub> emissions) can be used to track the age-of-air in the stratosphere.

# ff-CO<sub>2</sub>

Carbon Dioxide Emission Estimates from Fossil-Fuel Burning, Hydraulic Cement Production, and Gas Flaring for **1995** on a 1-deg x 1-deg Grid Cell Basis.

Antoinette L. Brenkert, CDIAC, Oak Ridge National Laboratory

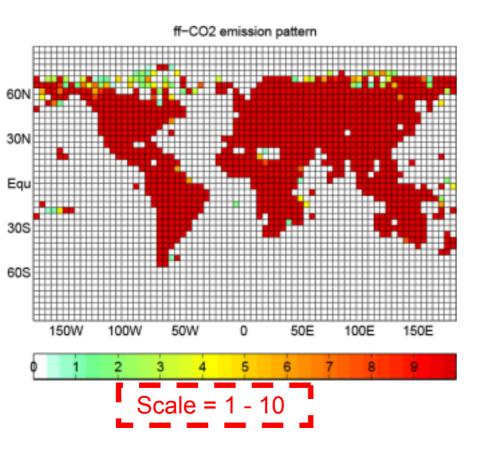


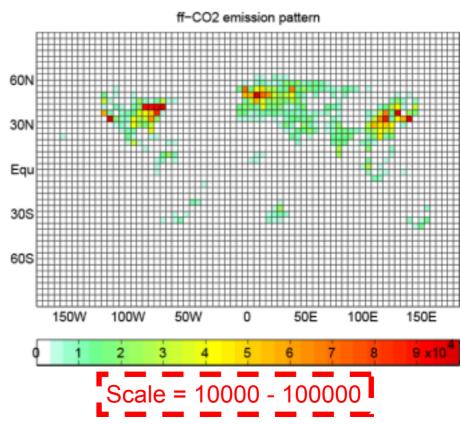
- initialize with zero fossil fuel CO<sub>2</sub>
- run for 10 years with 1995 ff-CO<sub>2</sub> emissions
- emissions scaled to 6.17 Tg-C/yr = 2.92 ppm/yr
- (slightly different from TransCom3: used 1990 → 1995)

### Fossil-Fuel CO<sub>2</sub> emission pattern:

1995 1°x1° emission pattern NDP-058A (2-1998) fossil-fuel burning, hydraulic cement prod. & gas flaring A.L. Brenkert, CDIAC

### >>>uniform emissions of 6.17 PgC/yr = 2.91 ppm/yr, no sinks<<<

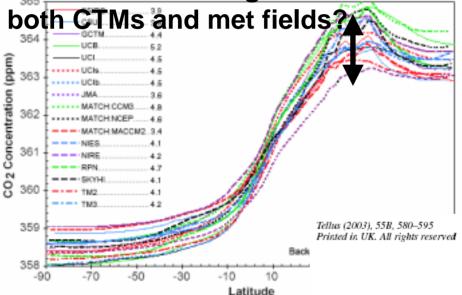




### TransCom 3 CO<sub>2</sub> inversion intercomparison: 1. Annual mean control results and sensitivity to transport and prior βux information

By KEVIN ROBERT GURNEY<sup>1</sup>, RACHEL M. LAW<sup>2</sup>, A. SCOTT DENNING<sup>1</sup>, PETER J. RAYNER<sup>2</sup>, DAVID BAKER<sup>3</sup>, PHILIPPE BOUSQUET<sup>4</sup>, LORI BRUHWILER<sup>5</sup>, YU-HAN CHEN<sup>6</sup>, PHILIPPE CIAIS<sup>4</sup>, SONGMIAO FAN<sup>2</sup>, INEZ Y. FUNG<sup>6</sup>, MANUEL GLOOR<sup>6</sup>, MARTIN HEIMANN<sup>6</sup>, KAZ HIGUCHI<sup>10</sup>, JASMIN JOHN<sup>8</sup>, EVA KOWALCZYK<sup>2</sup>, TAKASHI MAKI<sup>11</sup>, SHAMIL MAKSYUTOV<sup>12</sup>, PHILIPPE PEYLIN<sup>4</sup>, MICHAEL PRATHER<sup>13</sup>, BERNARD C. PAK<sup>13</sup>, JORGE SARMIENTO<sup>2</sup>, SHOICHI TAGUCHI<sup>14</sup>, TARO TAKAHASHI<sup>15</sup> and CHIU-WAI YUEN<sup>10</sup>

Can we reduce range that includes



Understanding the dispersion and mixing of fossil-fuel CO<sub>2</sub> is a critical element in inversions and understanding sources/sinks.

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Fig. 3. Annual mean, zonal mean surface CO<sub>2</sub> concentration (ppm) resulting a background concentration of 350 ppm) background Buses for each of the m for the background fossil and combined background CO<sub>2</sub> is listed in the key to for each of the plots.

TransCom 3 CO<sub>2</sub> inversion intercomparison: 2. Sensitivity of annual mean results to data choices

By RACHEL M. LAW1\*, YU-HAN CHEN2, KEVIN R. GURNEY3 and TRANSCOM 3 MODELLERS4,

8755-1209/02/2000RG000101\$15.00

1010. doi:10.1029/2000RG000101

### AGE OF STRATOSPHERIC AIR: THEORY, OBSERVATIONS, AND MODELS

Darryn W. Waugh Department of Earth and Planetary Sciences Johns Hopkins University Baltimore, Maryland, USA

Timothy M. Hall NASA Goddard Institute for Spa-

[1] We review the relationship between tracer distributions and transport timescales in the stratosphere and discuss the use of timescales to evaluate and constrain

theories and nur stratospheric air tracers, how see tion to constrain

"age spectrum," Tracking the observed falloff of vides a way to u stratospheric tracers like CO<sub>2</sub> and transport proces SF<sub>6</sub> has defined the age-of-air.

can be used to infer aspects of the age spectrum, most commonly the "mean age," but also the shape of the spectrum. Observational inferences of transport timescales provide stringent tests of numerical models independent of photochemistry, and comparisons of these observations with chemical transport models have highlighted certain problems with transport in the models. Age simulations and comparisons with data can now be considered standard tests of stratospheric models. INDEX

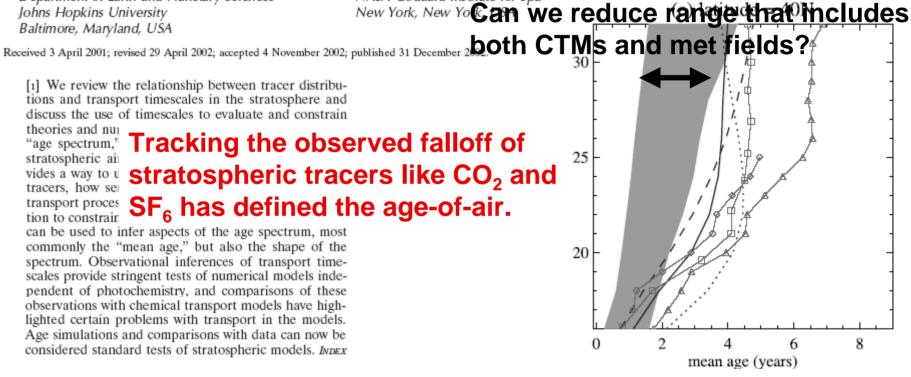


Figure 6. Comparison of observed (red curves with symbols) and modeled (blue shaded area and curves) mean age: (a) z = 20 km and latitude of (b) 5°S, (c) 40°N, and (d) 65°N. The shaded region indicates the range of most models in the Models and Measurements II (MM2) study, while the individual curves represent several models falling outside the range. The symbols represent observations: mean age from in situ CO<sub>2</sub> (diamonds) [Boering et al., 1996; Andrews et al., 2001b], in situ SF<sub>6</sub> (triangles) [Elkins et al., 1996; Ray et al., 1999], and whole air samples of SF<sub>6</sub> (square outside vortex and asterisk inside vortex) [Hamisch et al., 1996]. See Hall et al. [1999] for details. See color version of this figure at back of this issue.

### GMI study of accuracy in global tracer transport

use same GISS-2' 4°x5°x23-Layer met fields with GMI CTM and UCI CTM

#### Two basic simulations:

- A. 1hr / 3hr step (init f=1 in L=1 & 15, use Jan 1 21-24Z met fields)
- B. 10-year run with ff-CO2 emissions (init Jan 1 with f=0) (fossil-fuel emissions 1995 pattern, 6.17 Pg/yr = 2.92 ppm/yr)

#### Focus on:

- 1. Are we using the same met field (1 hr / 3 hr)
- 2. Stratospheric age-of-air (10-year run)
- 3. Surface and column CO<sub>2</sub> patterns (10-year run)

### Sensitivity studies:

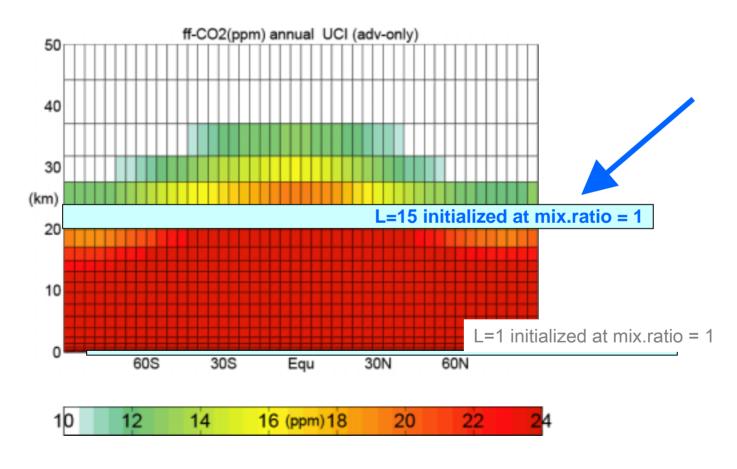
plus

Standard full run (std-A), Advection only (adv-E), Advection and BL-mixing only (ncnv-F) with GMI & UCI

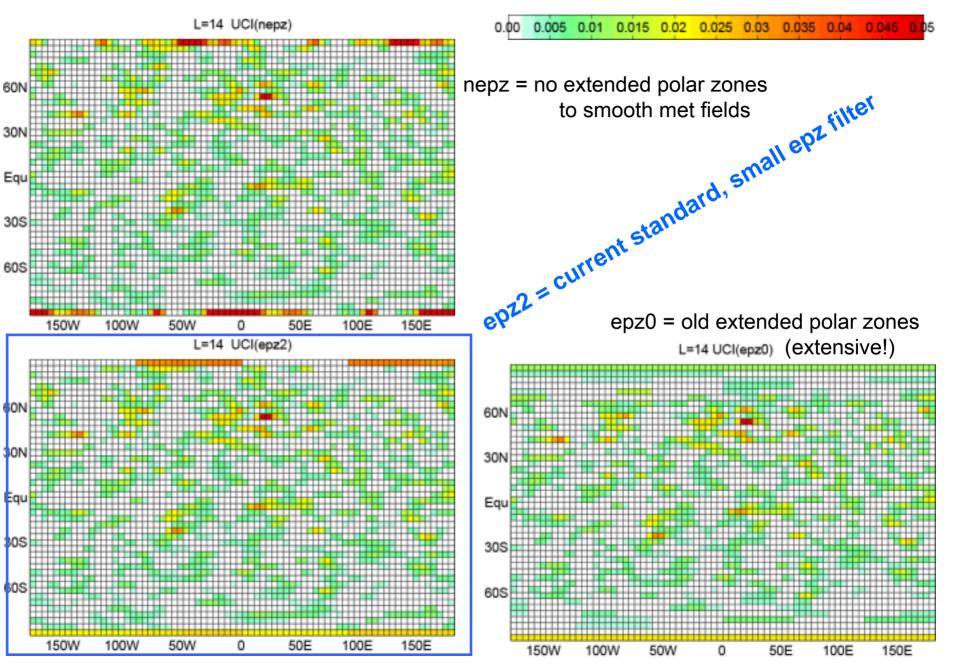
Different methods of BL mixing, convective entrainment, and averaging over extended polar zones with UCI only

### 1. The 1-hr / 3-hr Calculations:

look at pattern, amount advected from L=15 into L=14 & 16 use 'std' run (BL and convection did not impact L=14-15-16)

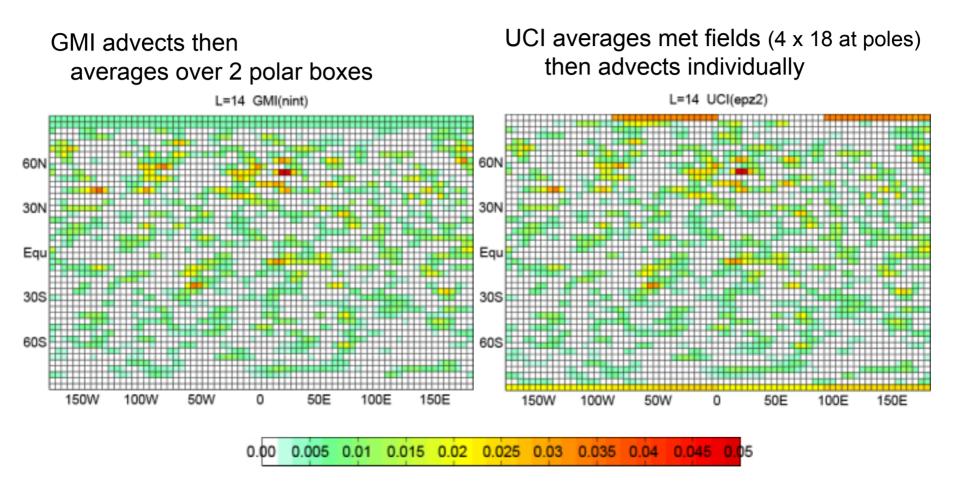


### Amount of tracer advected (f=1 @ L=15) to L=14 in 1 hr: UCI epz options

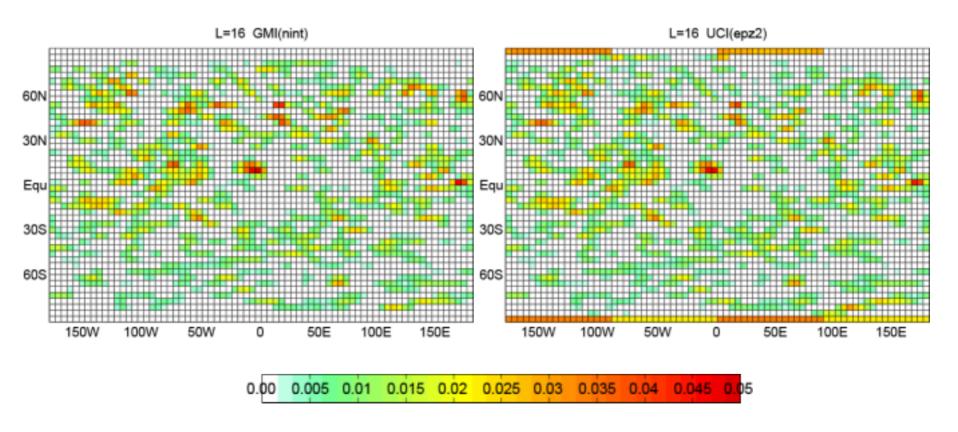


### Amount of tracer advected (f=1 at L=15) DOWN to L=14 in 1 hr: GMI vs. UCI

### GMI and UCI look very close, except at the poles



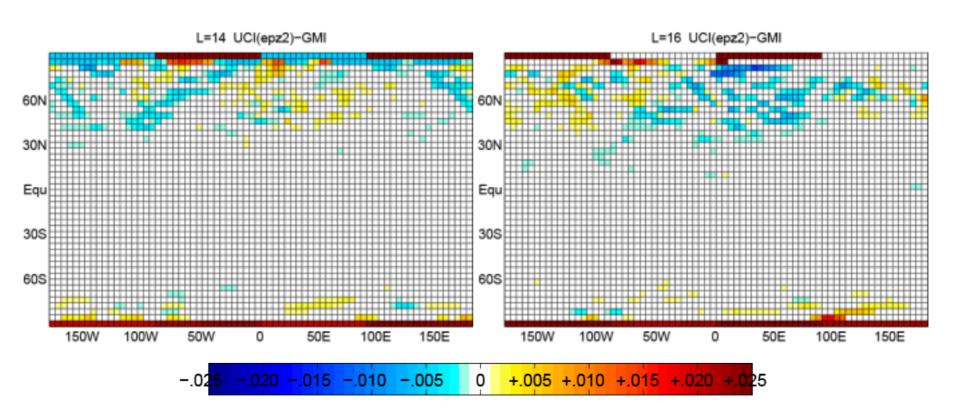
# Amount of tracer advected (f=1 at L=15) UP to L=16 in 1 hr: *GMI vs. UCI*GMI and UCI look very close, except at the poles



### Amount of tracer advected (f=1 at L=15) to L=14 & 16 in 1 hr: UCI - GMI

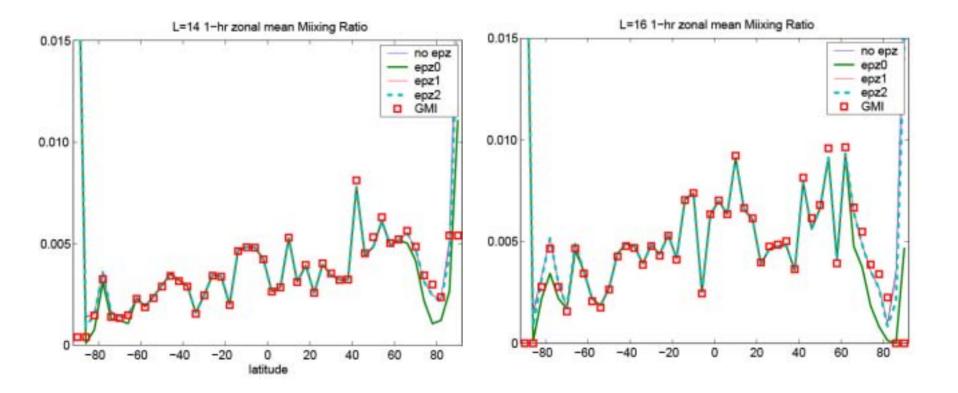
### GMI and UCI look very close, except at the poles

most errors small (±0.003) error pattern explained by (u,v,w) advection order (see next slide of zonal average\*\*)



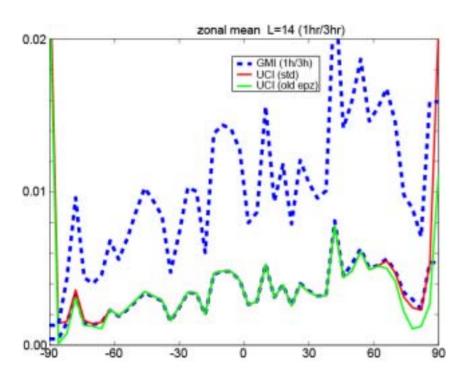
### Amount of tracer advected (f=1 at L=15) to L=14 & 16 in 1 hr: **zonal mean**

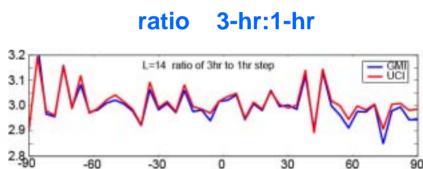
# zonally GMI and UCI are almost identical except at the poles\*\* (where UCI's old epz0 shows 'errors')



Amount of tracer advected (f=1 at L=15) to L=14 in 1 hr & 3 hr: zonal mean

# GMI and UCI both show anticipated 3-fold increase in L=14 after 3 hr AND have same zonal mean variation



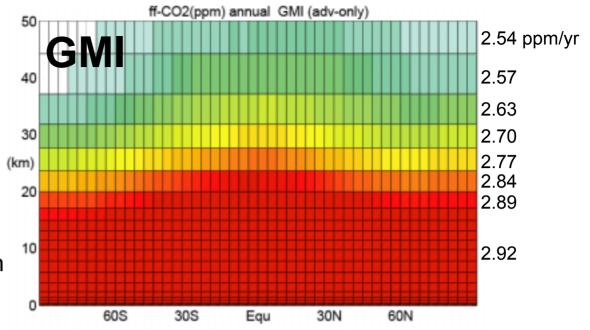


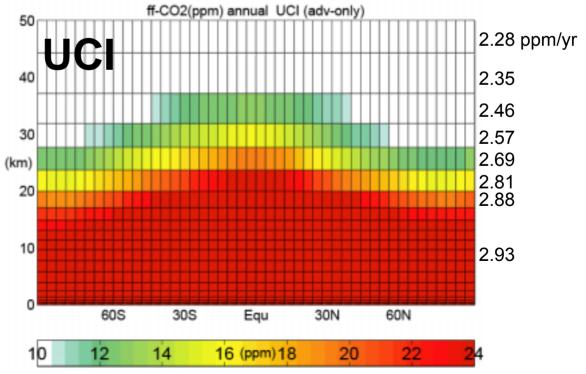
# 2. 10-yr runs for Stratospheric CO<sub>2</sub>

zonal mean CO<sub>2</sub> mixing ratio annual average of Year 10 actual model grid shown.

approach to steady-state shown as growth in Yr10

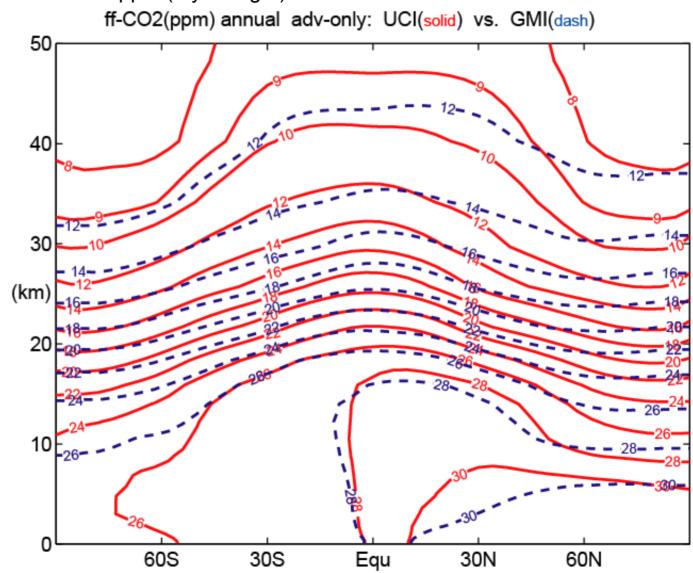
GMI vs. UCI (adv-only)
GMI is more "diffusive"
UCI is still 24% away from s-s



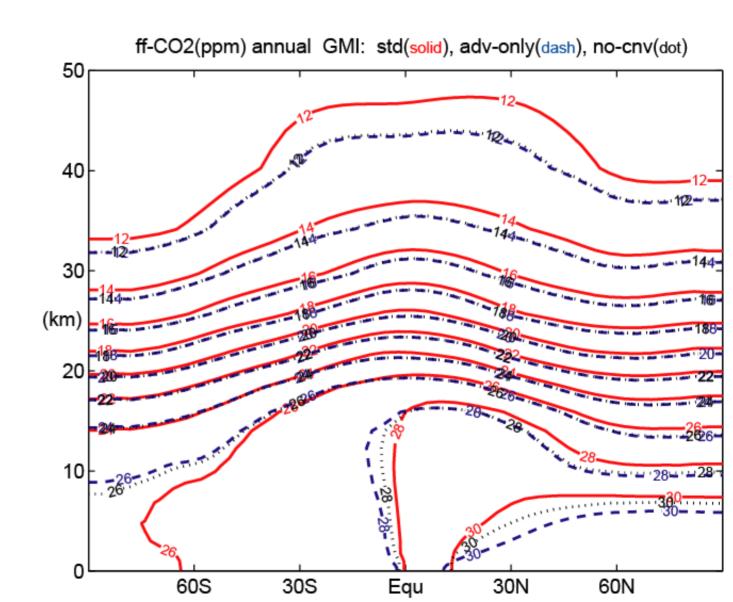


# GMI vs UCI CTM (adv-only)

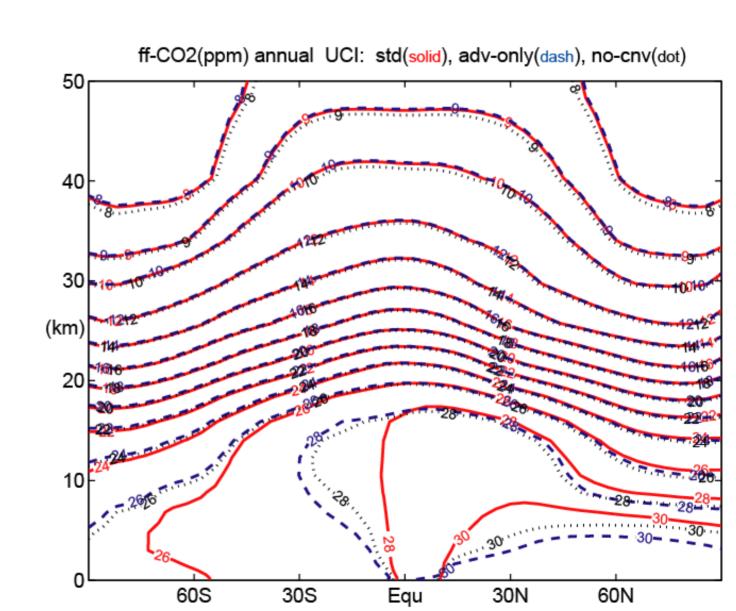
In lower tropics (20-28 ppm = 16-24 km) agreement is OK, but elsewhere GMI CTM cannot sustain vertical and horizontal gradients that UCI does GMI loses the poleward downward slope errors at 30 km are 2 to 4 ppm (1 yr in age!)



GMI appears to add some vertical diffusion (Kz) terms in the stratosphere? the std model mixes more vertically than adv-only or no-cnv



UCI shows almost no difference between std, adv-only and no-cnv but there is a worrying, small difference with no-cnv?



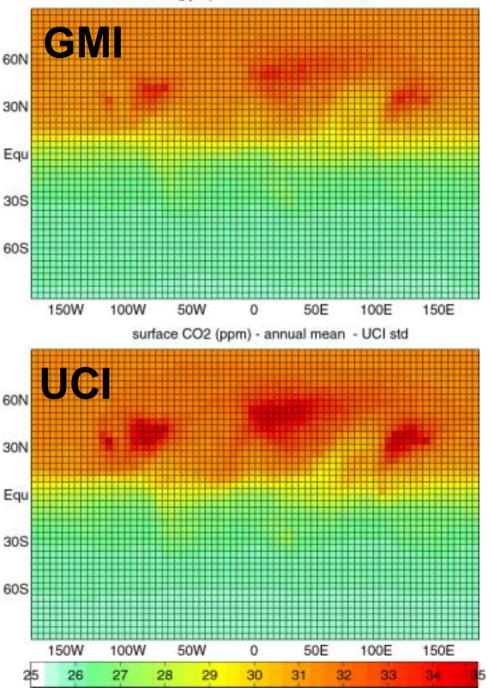
# 3. 10-yr runs for Trop. CO<sub>2</sub>

a. surface CO<sub>2</sub> mixing ratio &

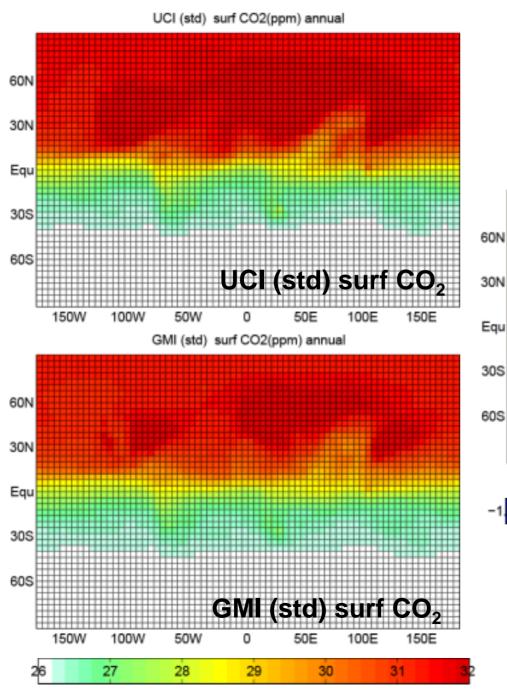
b. column CO<sub>2</sub> mixing ratio

annual or monthly means from Yr 10

GMI appears more "diffusive" UCI retains higher abundances over source regions.



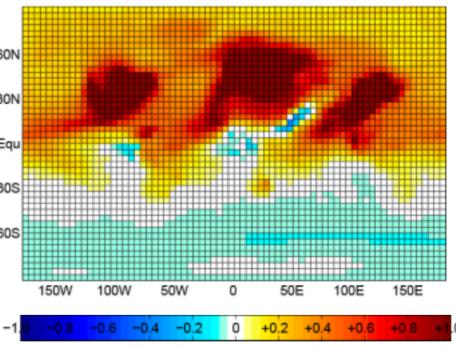
N.B. model 4x5 grid shown



### **SURFACE CO2**

### UCI - GMI





# Surface CO<sub>2</sub> - Annual mean:

# Compare UCI - GMI:

```
(std) = full, standard CTM with all processes
(ncnv) = advection + boundary-layer mix only
(adv) = advection only
```

+ (BL-up + noED) = UCI to look more like GMI

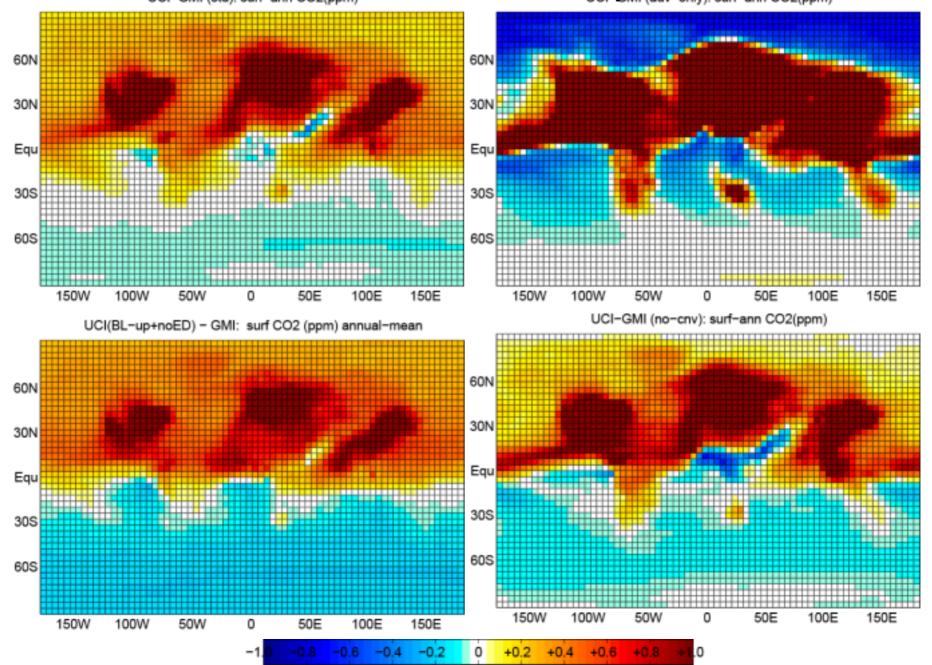
Compare UCI – GMI (std) with met-field differences:

GISS - DAO (GMI)

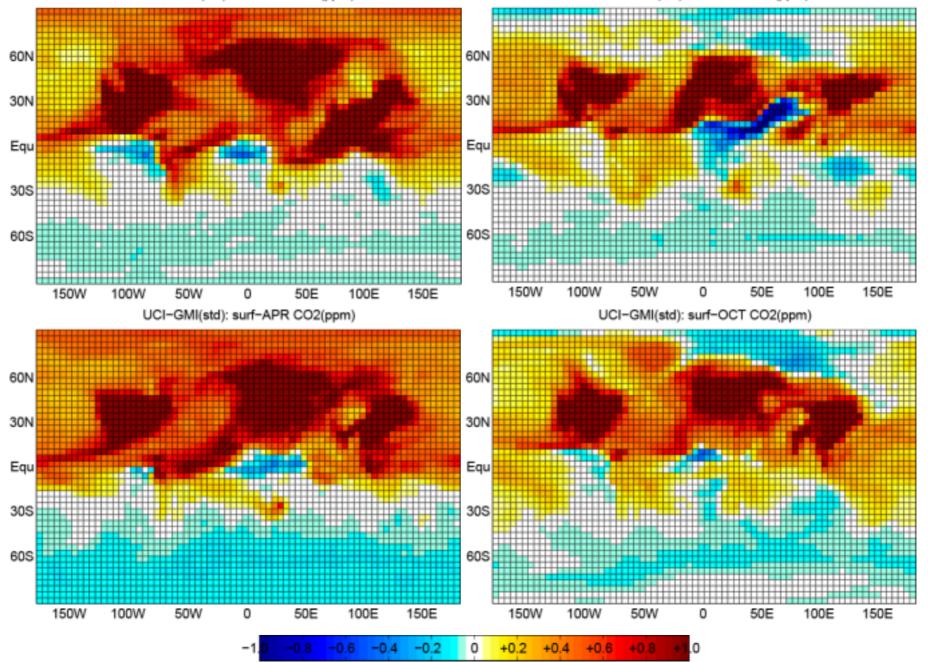
GISS – G78 (UCI, another 4x4x23L GISS met field)

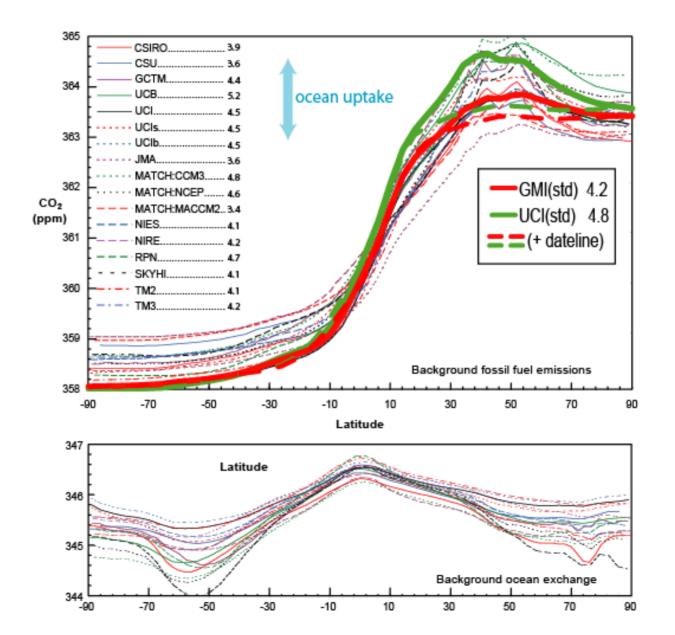
G77 – G78 (UCI, two consecutive years of G78)

UCI-GMI (std): surf-ann CO2(ppm) - GMI different components



UCI-GMI(std): surf-JAN CO2(ppm) UCI - GMI monthly UCI-GMI(std): surf-JUL CO2(ppm)





### Did not GMI solve this problem about the accuracy of the tracer transport?

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 104, NO. D22, PAGES 27,545-27,564, NOVEMBER 27, 1999

# Choosing meteorological input for the global modeling initiative assessment of high-speed aircraft

A. R. Douglass, M. J. Prather, T. M. Hall, S. E. Strahan, P. J. Rasch, L. C. Sparling, L. Coy, and J. M. Rodriguez

Abstract. The global modeling initiative (GMI) science team is developing a three-dimensional chemistry and transport model (CTM) for use in assessment of the atmospheric effects of aviation. This model must be documented, be validated against observations, use a realistic atmospheric circulation, and contain numerical transport and photochemical modules representing atmospheric processes. The

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 106, NO. D2, PAGES 1669-1691, JANUARY 27, 2001

Global Modeling Initiative assessment model.

Model description, integration, and testing

of the transport shell

- D. A. Rotman, J. R. Tannahill, D. E. Kinnison, P. S. Connell, D. Bergmann,
- D. Proctor, J. M. Rodriguez, S. J. Lin, R. B. Rood, M. J. Prather, 5
- P. J. Rasch,<sup>2</sup> D. B. Considine,<sup>6</sup> R. Ramaroson,<sup>7</sup> and S. R. Kawa<sup>4</sup>

Table 2. Summary Table of GMI Algorithms and Model Data

Module Options Input meteorological data NASA Data Assimilation Office (DAO) assimilated fields (NCAR MACCM2 GCM fields) NASA GISS II' GCM fields Advection algorithm semi-Lagrangian transport (SLT) (flux form semi-Lagrangian transport (FFSLT)) second-order moments (SOM) Mass tendencies (NASA GISS/University of California, Irvine, pressure filte Numerical schemes for chemistry solutions SMVGEAR II (semi-implicit syr N<sub>2</sub>O with GISS met fields & UCI S@M

Figure 4. Steady state zonal averaged N<sub>2</sub>O simulation results for January using the GMI model. (a) Results obtained using the GISS II' meteorological input data with the second-order moment method advection scheme. (b) Results obtained using the GISS II' meteorological input data with the flux form semi-Lagrangian advection scheme. Units are ppby.

N<sub>2</sub>O with GISS met fields & GMI tpcore

Latitude

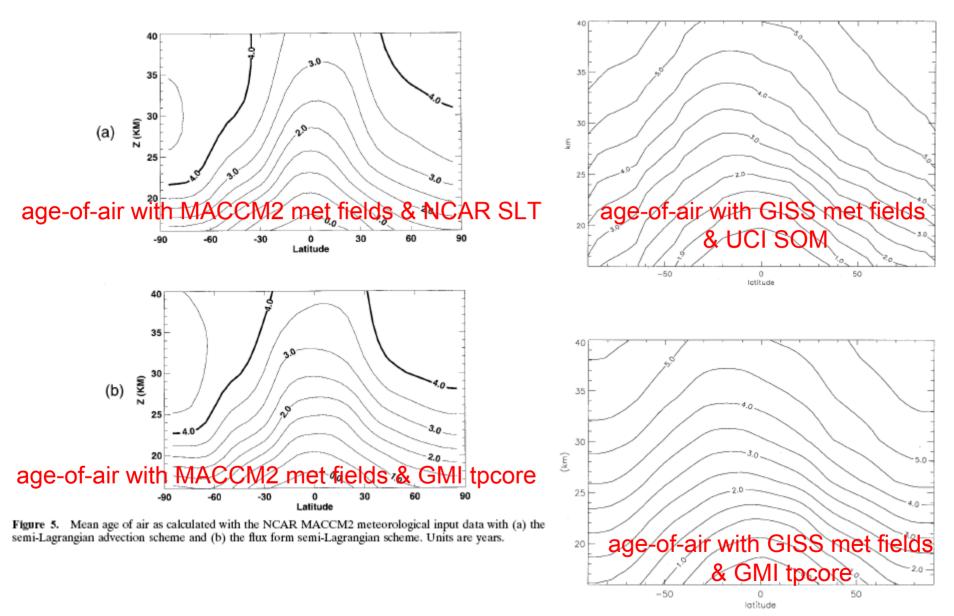


Figure 6. Mean age of air as calculated with the GISS II' meteorological input data with (a) the secondorder moment advection scheme and (b) the flux form semi-Lagrangian scheme. Units are years.

# UCI – GMI: 2x to convergence (1)

Assume: Differences between the UCI and GMI CTMs in the simple-tracer CO<sub>2</sub> experiments are due primarily to numerical error.

The numerical error is proportional to  $\triangle xyz$  (grid size).

Alternative: There are systematic errors in the two CTMs in either coding or basic algorithms. Let's not go there.

Let  $A(\Delta)$  be the CTM 'answer' computed with grid size  $\Delta$  have an error  $\epsilon(\Delta)$ 

$$A^{\text{true}} = A(\Delta \rightarrow 0) = A(\Delta) + \epsilon(\Delta)$$

# UCI – GMI: 2x to convergence (2)

$$A^{\text{true}} = A(\Delta \rightarrow 0) = A(\Delta) + \epsilon(\Delta)$$

$$A_1 = A(\Delta)$$

$$A_2 = A(\Delta/2)$$

When the order of the error (in terms of Taylor series expansion about  $\Delta$ ) is known, a simple approach with only two calculations (e.g., A( $\Delta$ ) and A( $\Delta$ /2)) can work:

Richardson extrapolation of trapezoidal integration ( $\epsilon \sim \Delta^2$ )

$$\varepsilon(\Delta) = a \Delta^2 + b \Delta^4 + \dots$$
  
$$\varepsilon(\Delta/2) = a/4 \Delta^2 + b' (\Delta/2)^4 + \dots$$

hence

$$4 A_2 - A_1 = 3 A^{true} + b'' \Delta^4 + \dots$$

and the error

$$\varepsilon(\Delta/2) = (A_2 - A_1)/3 + \operatorname{order}(\Delta^4)$$

# UCI – GMI: 2x to convergence (3)

For the CTM calculation, we do not know the order of the error in  $\Delta$  and hence we resort to Aitkens acceleration.

In this case we assume that the series obtained by successively better approximations by a  $\Delta$ -halving converges

Atrue = 
$$A(\Delta) + [A(\Delta/2) - A(\Delta)] + [A(\Delta/4) - A(\Delta/2)]$$
  
+  $[A(\Delta/8) - A(\Delta/4)] + \dots$   
=  $A_1 + (A_2 - A_1) + (A_4 - A_2) + (A_8 - A_4) + \dots$ 

assume each successive term is smaller than previous by factor  $k = (A_4 - A_2) / (A_2 - A_1)$ 

then

$$A^{\text{true}} = A_1 + (A_2 - A_1)x(1 + k + k^2 + k^3 + k^4 + \dots)$$
$$= A_1 + (A_2 - A_1) / (1 - k)$$

# UCI – GMI: 2x to convergence (4)

Note that we need the sequence  $A_1$ ,  $A_2$ , and  $A_4$ , but would like also to calculate  $A_8$  to check that the k-values are stable

$$(A_4 - A_2) / (A_2 - A_1)$$
 ?=?  $(A_8 - A_4) / (A_4 - A_2)$ 

# UCI – GMI: 2x to convergence (5)

At UCI we recoded the CTM to do automatic grid doubling. The method of interpolating has been checked / run for advection only thus far. (Advection is identified as the primary difference between UCI and GMI CTMs.) For advection we do not interpolate across different grid boxes, but merely sub-divide the advective fluxes equally across the halved grid boxes.

Using the GISS-II' 4x5 GMI met fields, grid =  $72(I) \times 46(J) \times 23(L)$  there are several experiments:

```
L1* = F1 = I1:J1:L1 = 72 x 46 x 23 = standard CTM run

L2* = 72 x 46 x 46

L4* = 72 x 46 x 92

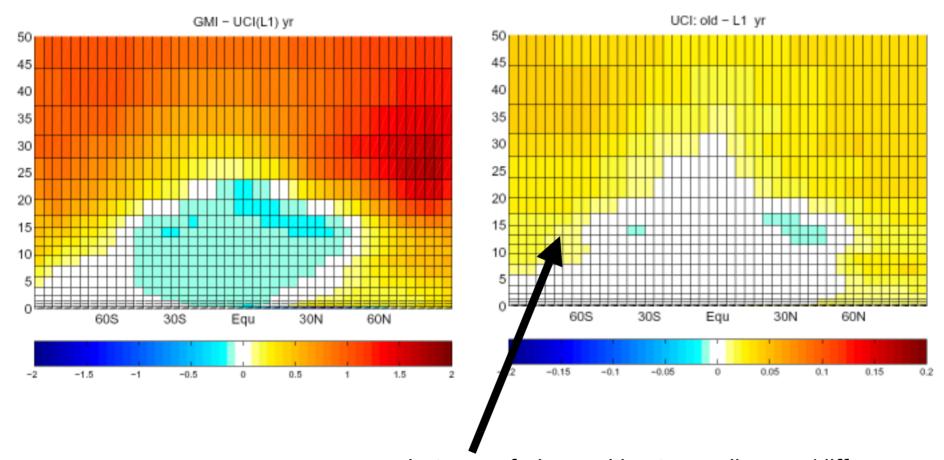
L8* = 72 x 46 x 184
```

<sup>\*10-</sup>yr run completed, \*\*run to 4 yr, \*\*\*run for only 2 months

### UCI – GMI: 2x to convergence (6)

- (1) Look at stratospheric age-of-air (L1=F1, L2, L4, L8, F2 10-yr runs)
- (2) Look at columns combination troposphere + stratosphere
- (3) Look at surface (L1, L2, L4, L8; F1, F2, F4 for year 1+)

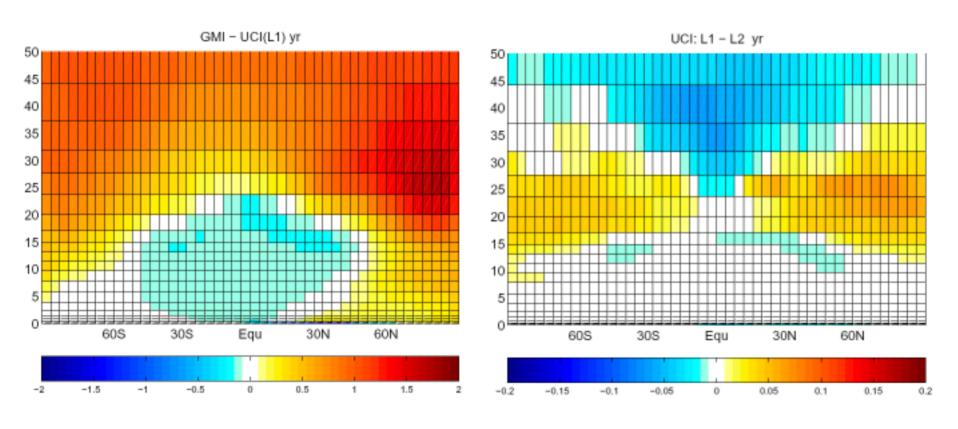
# UCI – GMI difference large, >1 yr over most of strat.



but age-of-air sensitive to small errors/differences in UCI code – NB different scale (0.05 vs 1) !!!

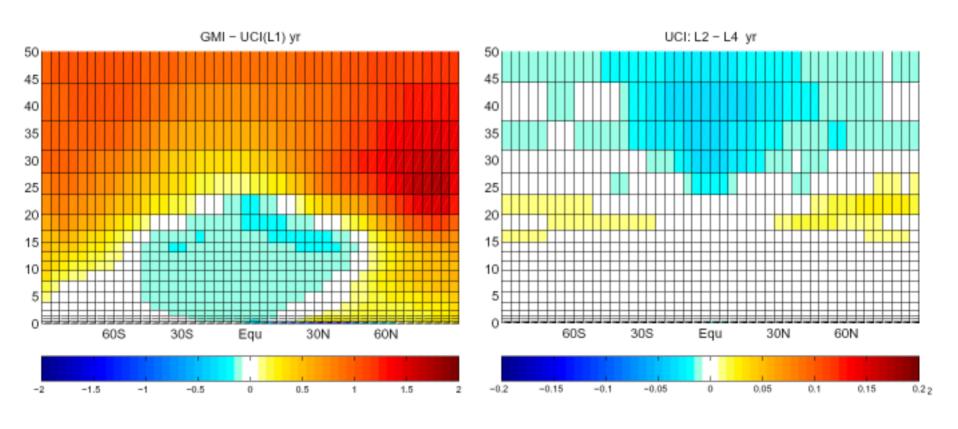
# UCI – GMI difference large, >1 yr over most of strat.

GMI-UCI vs. L1-L2, L2-L4, L4-L8. (different scales)



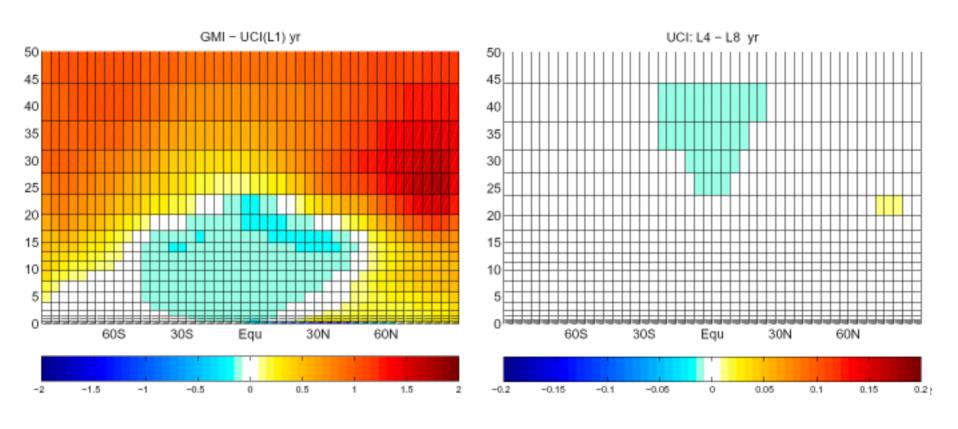
## UCI – GMI difference large, >1 yr over most of strat.

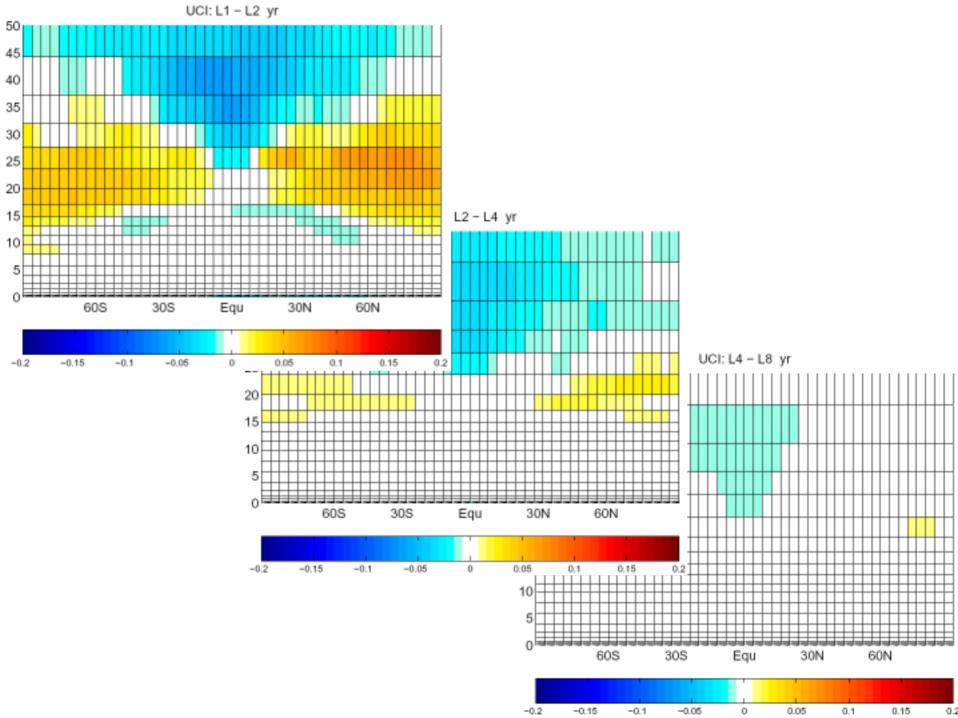
GMI-UCI vs. L1-L2, L2-L4, L4-L8. (different scales)

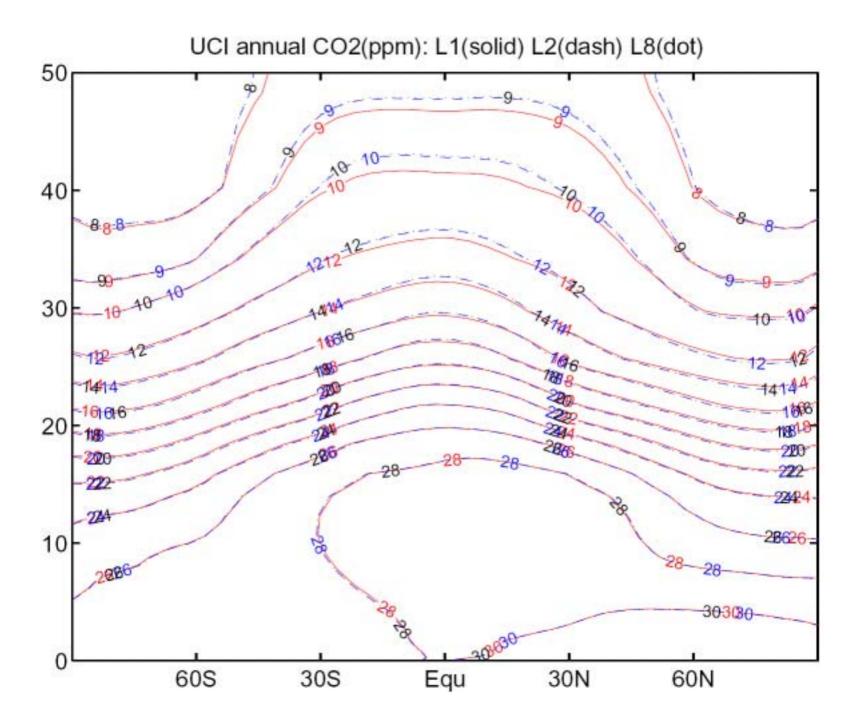


## UCI – GMI difference large, >1 yr over most of strat.

GMI-UCI vs. L1-L2, L2-L4, L4-L8. (different scales)







Ann L4 - L2 - F2 50 40 -100-10 30 744 166 12212 12122 18B8 1414 200 1444 222 16166 166 20 -244 #818° 244 1188 280 26 28626 200 2828 220 2222 -2222 244 -2224 10 26226= 2626-26 28-300-300 60S 30S 30N 60N Equ

# annual CO2(ppm): UCI-L1(solid) UCI-L2(dash) GMI(dot) 50 40 30 20 242624 10 30 30-30 60S 30S 30N 60N Equ

#### UCI – GMI: 2x to convergence (6)

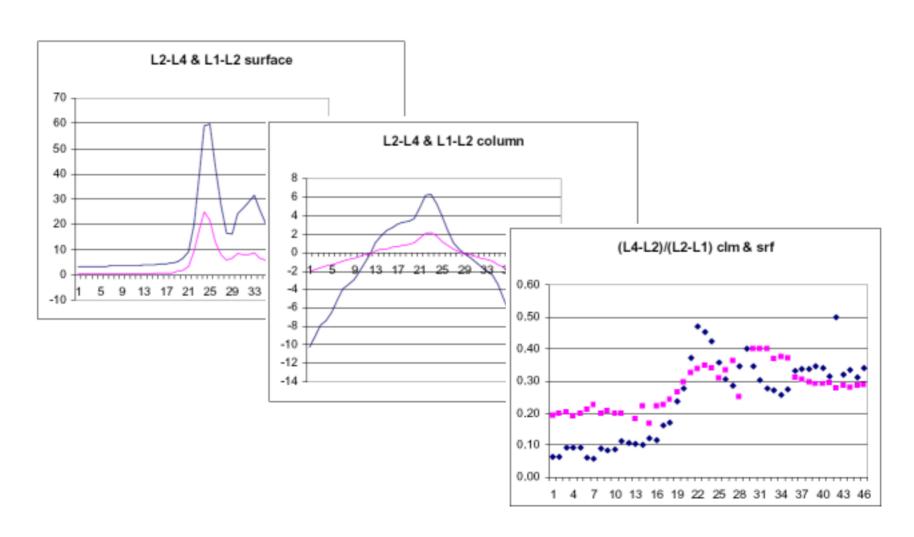
(1) Look at stratospheric age-of-air (L1=F1, L2, L4, L8, F2 10-yr runs)

#### (2) Look at columns – combination troposphere + stratosphere

(3) Look at surface (L1, L2, L4, L8; F1, F2, F4 for year 1+)

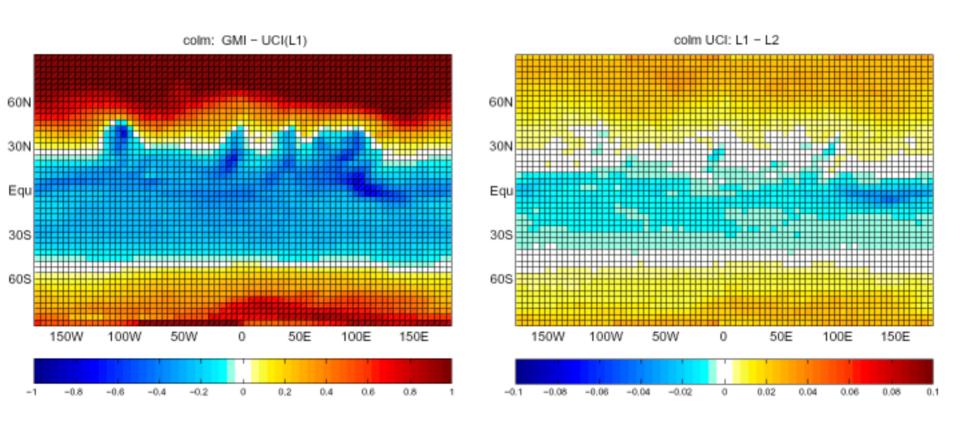
# Aitkens acceleration: looking at the sequence L1, L2, L4 for changes $(A_4 - A_2)$ and $(A_2 - A_1)$

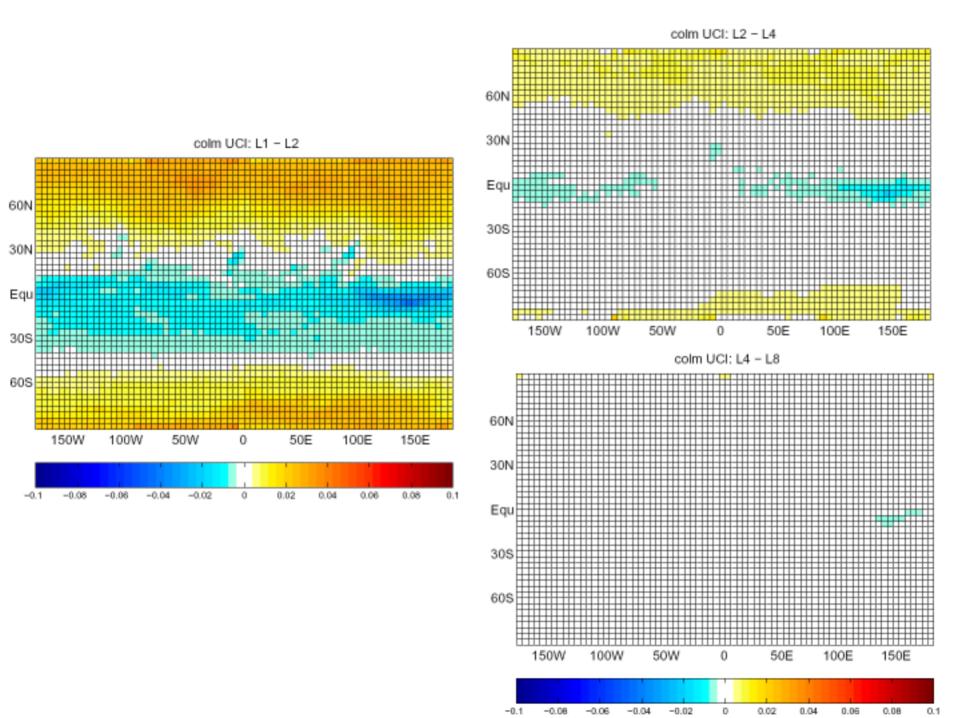
plots: zonal mean, yr 10, units = 0.001 ppm CO2 vs latitude J=1:46



#### UCI – GMI colm difference large.

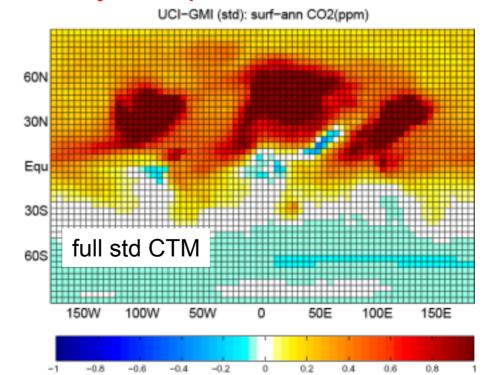
GMI-UCI vs. L1-L2, L2-L4, L4-L8. (different scales)



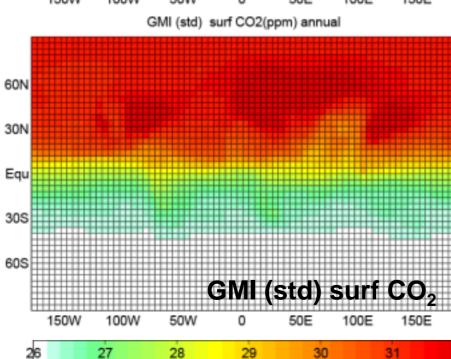


#### UCI – GMI: 2x to convergence (6)

- (1) Look at stratospheric age-of-air (L1=F1, L2, L4, L8, F2 10-yr runs)
- (2) Look at columns combination troposphere + stratosphere
- (3) Look at surface (L1, L2, L4, L8; F1, F2, F4 for year 1+)

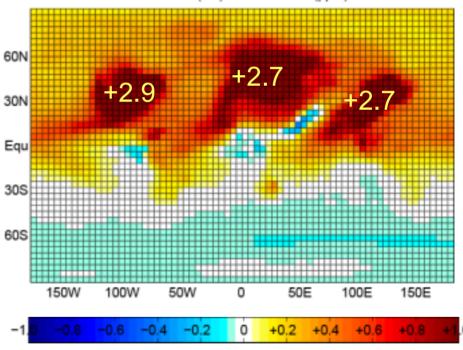


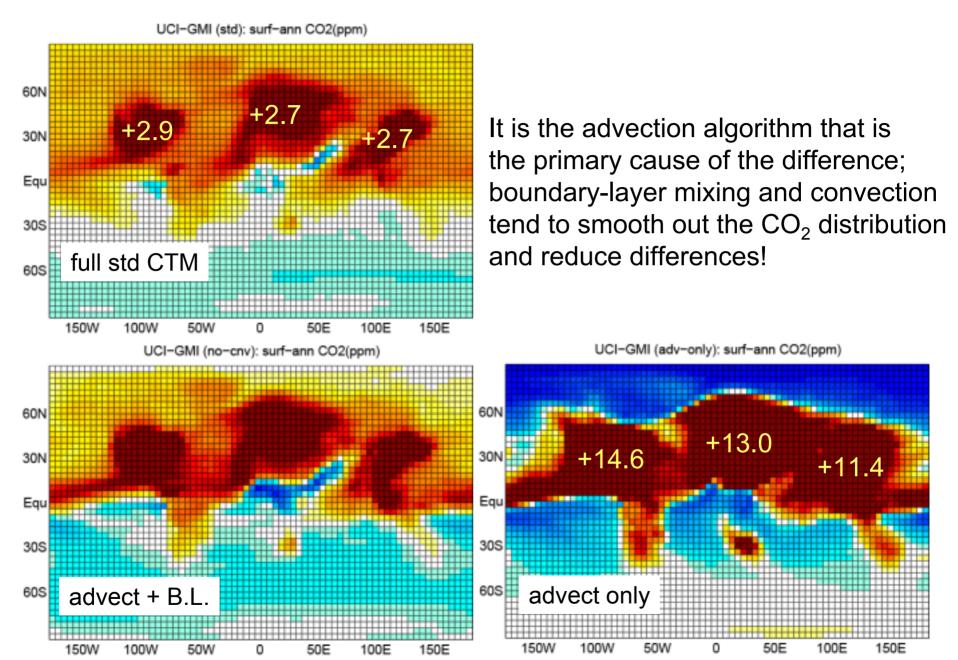
UCI (std) surf CO2(ppm) annual 60N 30N Equ 30S 60S UCI (std) surf CO<sub>2</sub> 100E 150W 100W 50W 150E GMI (std) surf CO2(ppm) annual

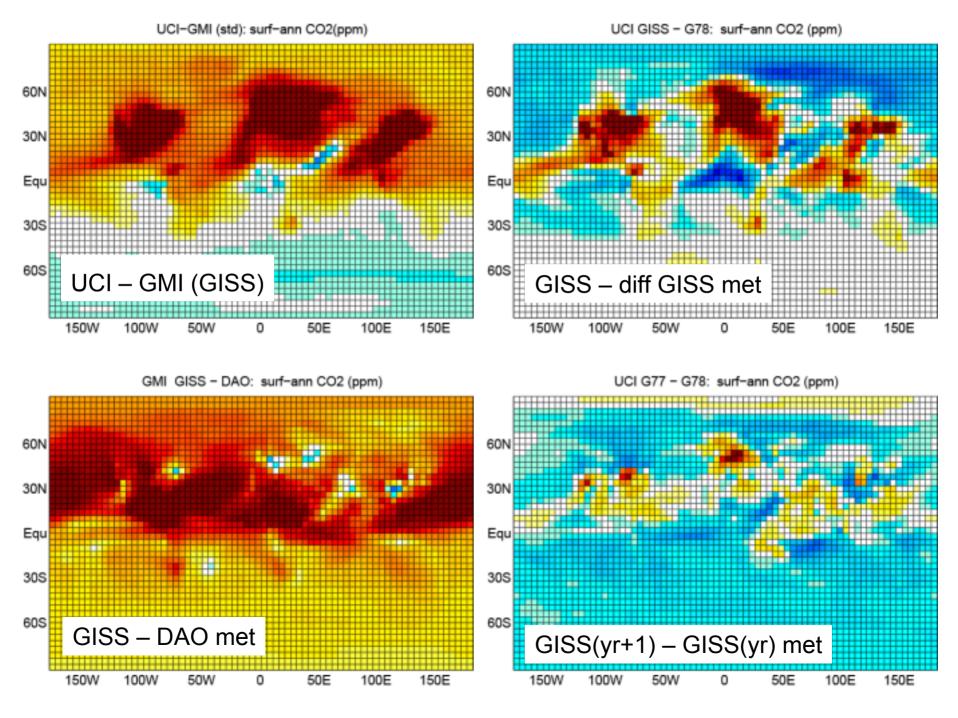


#### UCI - GMI









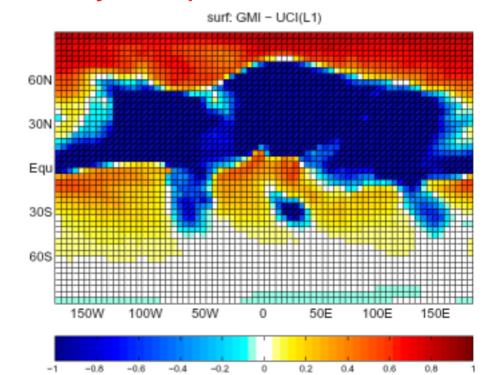
updated Mar 2004 – to correct some values, add the L1-L2-L4 converg, include rms var of total surface field.

 $CO_2$  difference at surface (r.m.s. of ann-mean,  $\langle N \rangle - \langle S \rangle = 4.5 ppm$ )

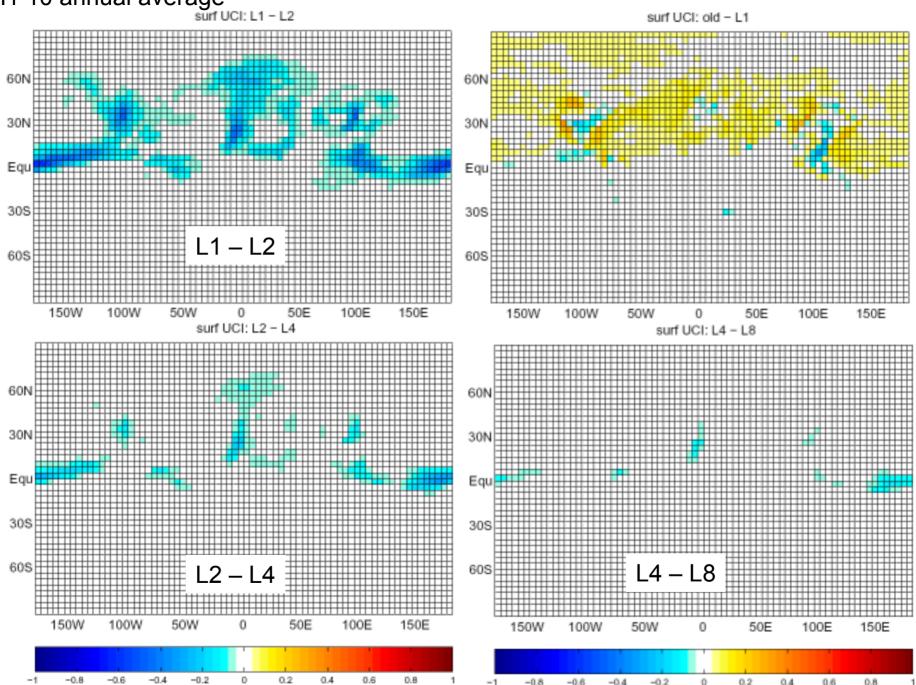
different CTMs (GISS met fields) UCI vs. GMI (std) – Feb'04 UCI (no ED, BL-up) vs. GMI (std) –better?	surf 0.55* ppm 0.47-0.45	rms var(UvG) 2.64 vs. 2.30
UCI vs. GMI (adv-only)	2.76	4.76 vs. 2.71
UCI vs. GMI (adv+BL)	0.67	2.71 vs. 2.26
different met fields (GMI & UCI CTMs)		
GISS vs. DAO	0.56 ppm	
GISS vs. G-78	0.32	
G-78 <sup>YR</sup> vs. G-78 <sup>YR+1</sup>	0.14	
different tunings (UCI CTM)		
Convection: no entrain/detrain	0.13	2.64
BL-mixing: 3-hr vs. instant	0.11	
BL round-up to whole layer vs. std	0.12	
Polar numerics: ext. polar zones	0.05	
Emissions: 1x1 w/SOM vs. 4x5	0.07	
Flux-limit: mono vs. pos-def	0.01	
GMI: press-error filters (LLNL vs. UCI)	0.04	
L1 – L2 (adv only)	<b>0.088</b> vs.	2.76 (UCI-GMI)
L2 – L4 (adv only)	0.036	

#### UCI – GMI: 2x to convergence (6)

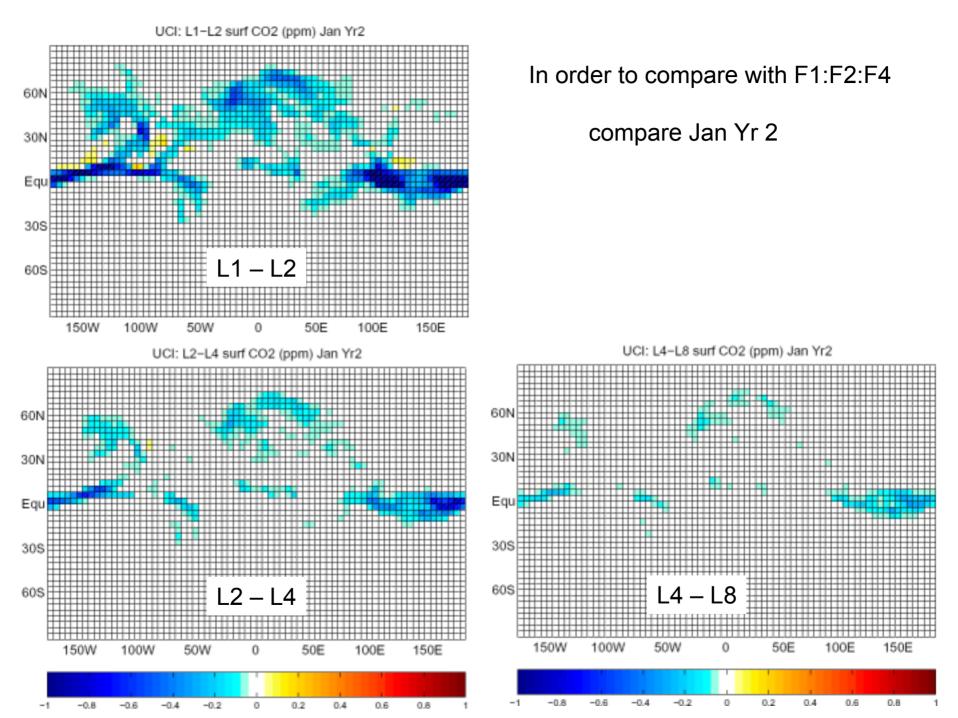
- (1) Look at stratospheric age-of-air (L1=F1, L2, L4, L8, F2 10-yr runs)
- (2) Look at columns combination troposphere + stratosphere
- (3) Look at surface (L1, L2, L4, L8; F1, F2, F4 for year 1+)

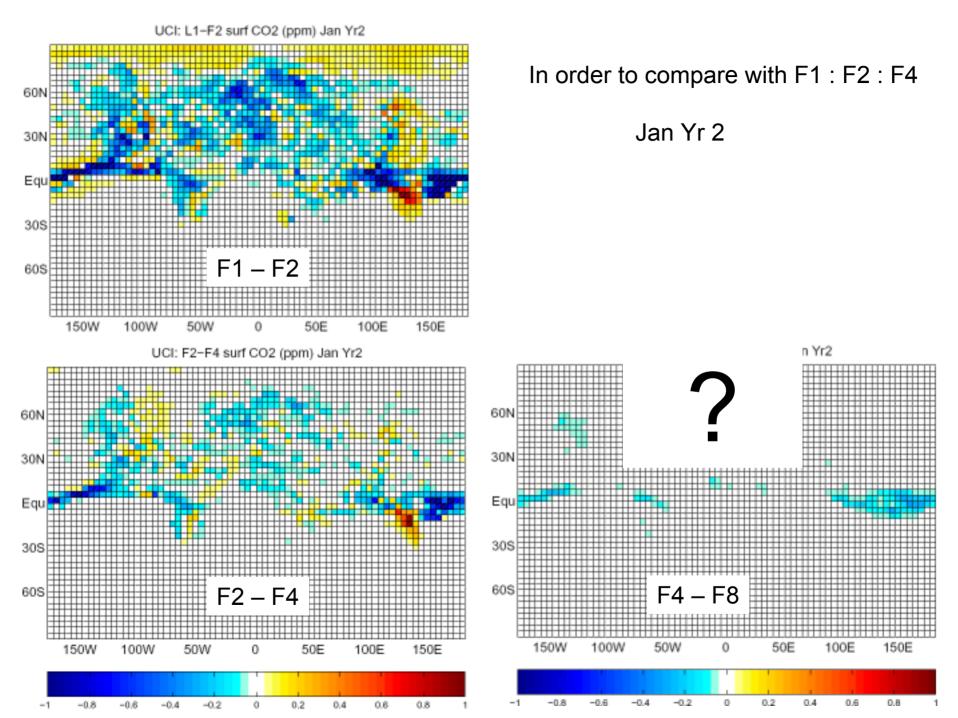


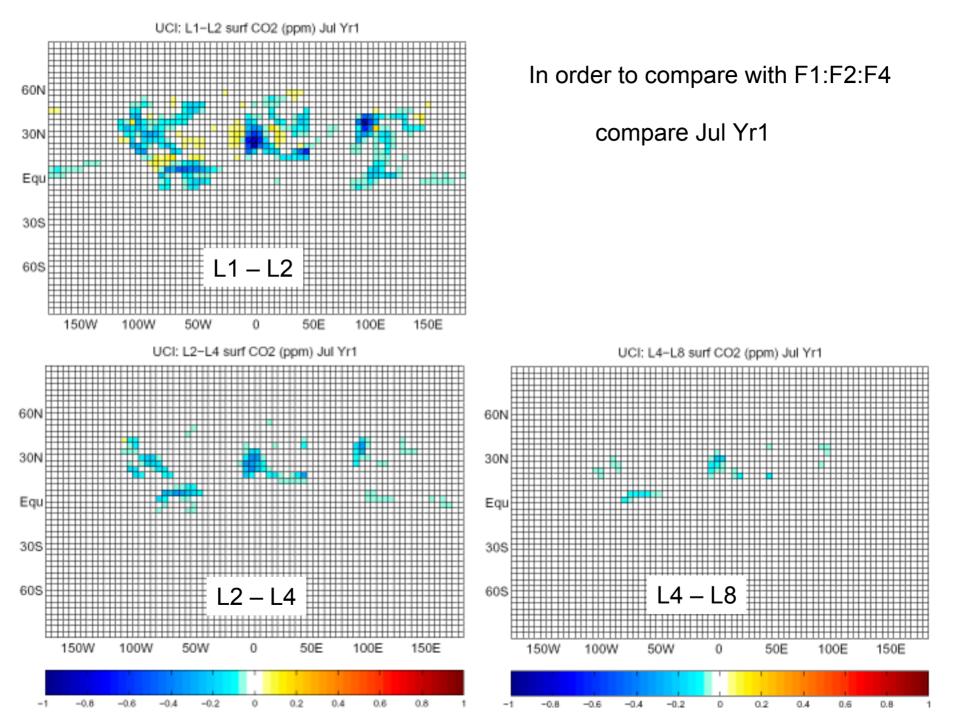
Yr 10 annual average surf UCI: L1 - L2

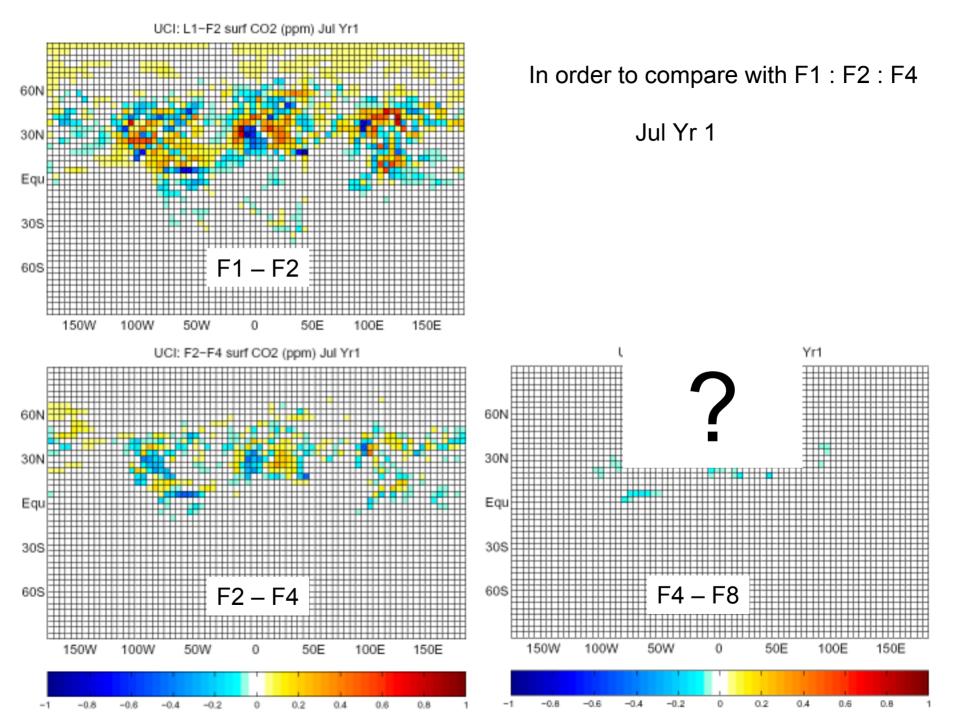


Yr 10 annual average surf UCI: L1 - L2 ratio (L4-L2)/(L2-L1) surface Y10 30N 30N Equ 308 30S ratio: (L4-L2)/(L2-L1) L1 - L2150W 100W 50W 50E 100E 150E 100E 150E surf UCI: L2 - L4 30N Equ L4 - L8100W 50W 50E 100E 150E 150W 100W 50W 50E 100E 150E







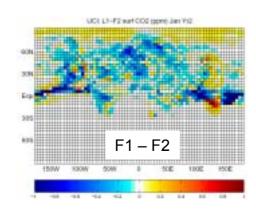


#### UCI – GMI: 2x to convergence (7)

Prospects look good. 2x is converging. F4 & F8 runs are getting difficult (F8 for trop only, 15 mon)

Looks like UCI CTM has error of about 0.2 ppm in strat ~0.1 yr → GMI CTM has error of ~1 yr

Surface errors in UCI CTM are large in places (1 ppm) but not as large as GMI-UCI diffs (~10 ppm)



#### UCI – GMI: 2x to convergence (8)

Propose GMI do the L1:L2:L4:L8 sequence.

The F1:F2:F4:F8 sequence requires VERY careful coding about the poles, not sure GMI can do it without significant effort.

-but it looks like the 2x2.5 and 4x5 cases could be redesigned

Could be a 'first' in proving CTMs converge to same answer. (Presumes that horizontal grid not a problem in stratosphere.)

Priorities? Aerosols and Trop, Chemistry still more important.